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FOR STOCHASTIC SYSTEMS

by

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LIKELIHOOD RATIO DERIVATIVE ESTIMATORS FOR STOCHASTIC SYSTEMS

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ABSTRACT

This paper discusses likelihood ratio derivative estimation techniques for stochastic systems. After a brief review of the basic concepts, likelihood ratio derivative estimators are presented for the following classes of stochastic processes: time homogeneous discrete-time Markov chains, non-time homogeneous discrete-time Markov chains, time homogeneous continuous-time Markov chains, semi-Markov processes, non-time homogeneous continuous-time Markov chains, and generalized semi-Markov processes.

1. INTRODUCTION

In recent years, an extensive literature has begun to develop within the simulation community on efficient estimation of derivatives of performance measures with respect to decision parameters. In this paper, we shall focus on describing the basic ideas that underlie a recently introduced derivative estimation method known as likelihood ratio derivative estimation (also known as the efficient score method). This technique has been previously described in GLYNN (1986, 1987), REIMAN and WEISS (1986), and RUBINSTEIN (1986).

In Section 2, we describe the basic likelihood ratio derivative estimator in a general setting in which the essential idea is most transparent. Section 3 specializes the estimator to discrete-time stochastic processes. We derive likelihood ratio derivative estimators for both time homogeneous and non-time homogeneous discrete-time Markov chains. In Section 4, we conclude the paper with a discussion of likelihood ratio derivative estimation in continuous time. We present, as examples of our analysis, the derivative estimators for: time homogeneous continuous-time Markov chains, non-time homogeneous continuous-time Markov chains, semi-Markov processes, and generalized semi-Markov processes. In all our examples, we require that the performance measure correspond to a terminating simulation.

As mentioned earlier, the likelihood ratio derivative estimation technique has been previously investigated in a number of different papers. Our main contribution here is

to specialize the general idea underlying this family of derivative estimators to the various classes of stochastic processes described above.

2. LIKELIHOOD RATIO DERIVATIVE ESTIMATION

In this section, we provide a brief introduction to the basic ideas that underlie likelihood ratio derivative estimation. To set the stage, consider a family of stochastic systems that is indexed by a scalar decision parameter θ . For example in a queueing context, θ might correspond to the service rate at a particular station. Given the sample space Ω , let $X(\theta, \omega)$ be the sample performance measure observed at sample outcome ω and decision parameter θ ; we permit $X(\theta, \omega)$ to depend explicitly on θ in order to encompass situations in which the "cost" of running the stochastic system (as measured through $X(\theta)$) depends on the parameter θ . (However, in many estimation settings, $X(\theta)$ is independent of θ and therefore depends only on ω .) In addition, the probability distribution P_θ on Ω typically depends on θ ; P_θ then reflects the manner in which the random environment is affected by the decision parameter. The performance measure $\alpha(\theta)$ associated with parameter value θ is then defined as the expectation

$$\alpha(\theta) = \int_{\Omega} X(\theta, \omega) P_\theta(d\omega).$$

Our goal is to describe an estimation methodology for calculating $\alpha'(\theta_0)$.

The likelihood ratio method for derivative estimation is based on the following idea. Suppose that there exists a measure μ (not necessarily a probability measure) such that $P_\theta(d\omega) = f(\theta, \omega)\mu(d\omega)$ i.e. $f(\theta, \cdot)$ is the density of P_θ with respect to μ . Then,

$$\alpha(\theta) = \int_{\Omega} X(\theta, \omega) f(\theta, \omega) \mu(d\omega).$$

Assuming that the derivative and integral can be interchanged, we obtain

$$\begin{aligned}\alpha'(\theta_0) &= \int_{\Omega} X'(\theta_0, \omega) f(\theta_0, \omega) \mu(d\omega) \\ &\quad + \int_{\Omega} X(\theta_0, \omega) f'(\theta_0, \omega) \mu(d\omega).\end{aligned}\quad (2.1)$$

We note that the first term on the right-hand side of (2.1) is just $E_{\theta_0} X'(\theta_0)$ (where $E_{\theta}(\cdot)$ denotes the expectation operator associated with P_{θ}). Since this term can be represented as the expectation of a r.v., standard Monte Carlo methods may be applied to estimate it. Specifically, suppose that one simulates i.i.d. replicates of $X'(\theta_0)$ under distribution P_{θ_0} ; the sample mean of these observations then converges (at rate $n^{-1/2}$ in the number n of observations) to the first term.

To handle the second term using Monte Carlo methods, we need to represent it as the expectation of a r.v. To accomplish this, suppose that $g(\omega)$ is a non-negative function such that

$$\int_{\Omega} g(\omega) \mu(d\omega) = 1. \quad (2.2)$$

Then, the measure $P(d\omega) = g(\omega) \mu(d\omega)$ is a probability distribution on Ω . If g has the additional property that

$$\begin{aligned}|X(\theta_0, \omega) f'(\theta_0, \omega)| &> 0 \text{ implies} \\ \text{that } g(\omega) &> 0,\end{aligned}\quad (2.3)$$

then we can represent the second term as

$$\int_{\Omega} X(\theta_0, \omega) \frac{f'(\theta_0, \omega)}{g(\omega)} g(\omega) \mu(d\omega) = E[X(\theta_0) H(\theta_0)] \quad (2.4)$$

where $H(\theta_0, \omega) = f'(\theta_0, \omega)/g(\omega)$ and $E(\cdot)$ denotes expectation relative to the probability P . (Note that (2.3) is required to avoid dividing by zero in (2.4).) Given the representation (2.4) of the second term as an expectation, we can now easily apply Monte Carlo methods to estimate it (in the same way as for the first term).

We now turn to the question of selecting the sampling density g . The theory of importance sampling asserts that the choice of g which minimizes the variance of the observations of $X(\theta_0) H(\theta_0)$ is

$$g^*(\omega) = \frac{|X(\theta_0, \omega) f'(\theta_0, \omega)|}{\int_{\Omega} |X(\theta_0, \omega) f'(\theta_0, \omega)| \mu(d\omega)}, \quad (2.5)$$

see GLYNN and IGLEHART (1989) for further details. Unfortunately, the optimal sampling density g^* basically requires knowledge of the integral (appearing in the second term in (2.1)) that we are trying to estimate. Therefore, the choice of g^* as defined by (2.5) is typically impractical to implement.

We now describe a popular alternative to g^* . Suppose that the densities $f(\theta, \omega)$ are such that for θ in an open neighborhood of θ_0 ,

$$\Lambda(\theta) = \{\omega : f(\theta, \omega) > 0\} \text{ is independent of } \theta. \quad (2.6)$$

Then, $f(\theta_0, \omega) = 0$ implies that $f(\theta, \omega)$ vanishes in a neighborhood of θ , from which it follows that $f'(\theta_0, \omega) = 0$, so that $f'(\theta_0, \omega) X(\theta_0, \omega) = 0$. Thus, $g(\omega) = f(\theta_0, \omega) \mu(d\omega)$ satisfies both (2.2) and (2.3). In this case,

$$H(\theta_0, \omega) = \frac{f'(\theta_0, \omega)}{f(\theta_0, \omega)} \left(= \frac{d}{d\theta} \log f(\theta_0, \omega) \right); \quad (2.7)$$

the right-hand side of (2.7) is known as the likelihood ratio derivative (because $H(\theta_0, \omega) = \frac{d}{d\theta} \frac{f(\theta, \omega)}{f(\theta_0, \omega)}$ is the derivative of the quantity known in the statistics literature as the likelihood ratio of P_{θ} with respect to P_{θ_0}).

This choice of g has an important advantage. Note that if we sample outcomes ω according to $f(\theta_0, \omega) \mu(d\omega)$, we can use the c.v.'s $X(\theta_0)$, $X'(\theta_0)$, and $X(\theta_0) H(\theta_0)$ to estimate $\alpha(\theta_0)$ and both the terms appearing on the right-hand side of (2.1) simultaneously. Thus, with this choice of g , we may estimate $\alpha(\theta_0)$ and $\alpha'(\theta_0)$ using the original sampling distribution associated with parameter θ_0 . At the same time, it should be noted that there are important problem classes (e.g. rare event simulations) in which much better choices of g can be made (better in the sense of smaller variance).

We close this section by recalling that to derive (2.1), an interchange of the differentiation and expectation operators was required. In virtually all practical examples, the interchange is valid under mild additional regularity assumptions on the problem. As a consequence, we shall ignore this interchange issue throughout the remainder of this paper.

3. LIKELIHOOD RATIO DERIVATIVE ESTIMATION IN DISCRETE TIME

In this section, we specialize the discussion of Section 2 to the case where $X(\theta, \omega)$ is a sample performance measure

associated with a discrete-time sequence $Y = (Y_n : n \geq 0)$ taking values in a discrete state space S . Specifically, we suppose that $\Omega = S \times S \times \dots$ and that Y_n is the coordinate r.v. $Y_n(\omega) = \omega_n$ for $\omega = (\omega_0, \omega_1, \dots) \in \Omega$. We assume that $X(\theta)$ takes the form

$$X(\theta) = h(\theta, Y_0, Y_1, \dots),$$

for some real-valued function h . Since S is discrete, there exist joint probability mass functions p_0, p_1, \dots such that

$$P_\theta\{Y_0 = y_0, \dots, Y_n = y_n\} = p_n(\theta, \bar{y}_n) \quad (3.1)$$

where $\bar{y}_n = (y_0, \dots, y_n)$. Letting

$$\begin{aligned} & p_n(\theta, \bar{y}_{n-1}; y_n) \\ &= P_\theta\{Y_n = y_n | Y_0 = y_0, \dots, Y_{n-1} = y_{n-1}\}, \end{aligned}$$

we can write (3.1) as the product

$$\begin{aligned} & P_\theta\{Y_0 = y_0, \dots, Y_n = y_n\} \\ &= p_0(\theta, y_0) \prod_{k=0}^{n-1} p_k(\theta, \bar{y}_k; y_{k+1}) \end{aligned}$$

Suppose now that $X(\theta)$ is a function of Y up to some finite (deterministic) time horizon m , so that $X(\theta) = h(\theta, \bar{Y}_m)$ where $\bar{Y}_m = (Y_0, \dots, Y_m)$. To apply the idea of Section 2, we need to obtain a representation $P_\theta(d\omega) = f(\theta, \omega)\mu(d\omega)$ for some measure μ . But observe that for $\omega \in \Omega_m$,

$$P_\theta(d\omega) = p_\theta(\theta; \omega_0) \prod_{k=0}^{n-1} p_k(\theta, \bar{\omega}_k; \omega_{k+1}) \mu_m(d\omega)$$

$\bar{\omega}_k = (\omega_0, \dots, \omega_k)$ and μ_m is counting measure on $\Omega_m = S \times S \times \dots \times S$ ($m + 1$ times). Hence, we may take

$$f(\theta, \omega) = p(\theta, \omega_0) \prod_{k=0}^{m-1} p(\theta, \bar{\omega}_k; \omega_{k+1}),$$

so that

$$\begin{aligned} f'(\theta_0, \omega) &= p'(\theta_0, \omega_0) \prod_{k=0}^{m-1} p_k(\theta_0, \bar{\omega}_k; \omega_{k+1}) \\ &+ p(\theta_0, \omega_0) \sum_{k=0}^{m-1} p'_k(\theta_0, \bar{\omega}_k; \omega_{k+1}) \prod_{j \neq k} p_j(\theta_0, \bar{\omega}_j; \omega_{j+1}). \end{aligned} \quad (3.3)$$

We can simplify the above formula somewhat. We claim that if $p'_k(\theta_0, \bar{\omega}_k; \omega_{k+1}) \neq 0$, it must follow that $p_k(\theta_0, \bar{\omega}_k; \omega_{k+1}) > 0$. For suppose that $p_k(\theta_0, \bar{\omega}_k; \omega_{k+1}) = 0$. Then it follows that

$$p_k(\theta_0 + h, \bar{\omega}_k; \omega_{k+1}) = p'_k(\theta_0, \bar{\omega}_k; \omega_{k+1})h + o(h)$$

as $h \downarrow 0$, from which it is evident that $p_k(\theta_0 + h, \bar{\omega}_k; \omega_{k+1}) < 0$ for some h . But $p_k(\theta, \bar{\omega}_k; \omega_{k+1})$ is a mass function and hence must be non-negative. This contradiction guarantees that $p_k(\theta_0, \bar{\omega}_k; \omega_{k+1}) > 0$. A similar argument shows that $p_0(\theta_0, \omega_0) > 0$ whenever $p'_0(\theta_0, \omega_0) \neq 0$. Hence, we may write (3.3) as

$$f'(\theta_0, \omega) = f(\theta_0, \omega) \left[\frac{p'_0(\theta_0, \omega_0)}{p_0(\theta_0, \omega_0)} + \sum_{k=0}^{m-1} \frac{p'_k(\theta_0, \bar{\omega}_k; \omega_{k+1})}{p_k(\theta_0, \bar{\omega}_k; \omega_{k+1})} \right]$$

Suppose that we choose a g such that $\int_{\Omega_m} g(\omega) \mu_m(d\omega) = 1$ and $f(\theta_0, \omega) > 0$ implies that $g(\omega) > 0$; then (2.3) is automatically in force. (In particular, setting $g(\omega) = f(\theta_0, \omega)$ works.) Hence, we find that

$$\alpha'(\theta_0) = E_g X'(\theta_0) + E_g X(\theta_0) H(\theta_0) \quad (3.4)$$

where $E_g(\cdot)$ denotes the expectation operator associated with the probability $P_g(d\omega) = g(\omega) \mu_m(d\omega)$, $E_\theta(\cdot)$ denotes expectation relative to P_θ , and

$$H(\theta_0) = \frac{f(\theta_0, \bar{Y}_m)}{g(\bar{Y}_m)} \left[\frac{p'_0(\theta_0, Y_0)}{p_0(\theta_0, Y_0)} + \sum_{k=0}^{m-1} \frac{p'_k(\theta_0, \bar{Y}_k; Y_{k+1})}{p_k(\theta_0, \bar{Y}_k; Y_{k+1})} \right].$$

The same argument can be extended to a certain class of random time horizons. In particular, suppose that T is

a stopping time with respect to Y i.e. for each $m \geq 0$, $I(T = m) = k_m(\vec{Y}_m)$ for some function k_m . We assume that the performance measure $X(\theta)$ is a function of the path of Y up to the random time horizon T i.e. there exists a family of functions h_0, h_1, \dots such that

$$\begin{aligned} X(\theta) &= \sum_{m=0}^{\infty} h_m(\theta, \vec{Y}_m) I(T = m) \\ &= h_T(\theta, \vec{Y}_T) I(T < \infty). \end{aligned} \quad (3.5)$$

As in the derivation of (3.4), we need to represent P_θ as $P_\theta(d\omega) = f(\theta, \omega)\mu(d\omega)$. Let $\Omega_T = \cup_{m=0}^{\infty}\{\vec{\omega}_m \in \Omega_m : k_m(\vec{\omega}_m) = 1\}$ and note that for $\omega = (\omega_0, \omega_1, \dots, \omega_T) \in \Omega_t$,

$$\begin{aligned} P_\theta(d\omega) &= \\ p_0(\theta, \omega_0) \prod_{k=0}^{T-1} p_k(\theta, \vec{\omega}_k; \omega_{k+1}) \mu_T(d\omega) \end{aligned} \quad (3.6)$$

where μ_T is counting measure on Ω_T . Suppose that g is chosen as a non-negative function on Ω_T having the property that $\int_{\Omega} g(\omega) \mu_T(d\omega) = 1$ and $p_0(\theta_0, \omega_0) \prod_{k=0}^{T-1} p_k(\theta_0, \vec{\omega}_k; \omega_{k+1}) > 0$ implies that $g(\omega) > 0$ for $\omega \in \Omega_T$. By combining (3.5) and (3.6) and proceeding as in the derivation of (3.4), we obtain the following stopping time generalization of (3.4):

$$\alpha'(\theta_0) = E_{\theta_0} X'(\theta_0) + E_g X(\theta_0) H(\theta_0) \quad (3.7)$$

where

$$\begin{aligned} H(\theta_0) &= \frac{p_0(\theta_0, Y_0) \prod_{k=0}^{T-1} p_k(\theta_0, \vec{Y}_k; Y_{k+1})}{g(\vec{Y}_T)} \\ &\left[\frac{p'_0(\theta_0, Y_0)}{p_0(\theta_0, Y_0)} + \sum_{k=0}^{T-1} \frac{p'_k(\theta_0, \vec{Y}_k; Y_{k+1})}{p_k(\theta_0, \vec{Y}_k; Y_{k+1})} \right]. \end{aligned}$$

As in the case of (3.4), one possible choice of g is $f(\theta_0)$, in which event (3.7) simplifies to:

$$\alpha'(\theta_0) = E_{\theta_0} [X'(\theta_0) + X(\theta_0) H(\theta_0)] \quad (3.8)$$

where

$$H(\theta_0) = \frac{p'_0(\theta_0, Y_0)}{p_0(\theta_0, Y_0)} + \sum_{k=0}^{T-1} \frac{p'_k(\theta_0, \vec{Y}_k; Y_{k+1})}{p_k(\theta_0, \vec{Y}_k; Y_{k+1})}.$$

We now give a couple of examples to illustrate (3.7) and (3.8).

(3.9) EXAMPLE. Suppose that under distribution P_θ , Y is a Markov chain with initial distribution $\mu(\theta)$ and transition matrix $P(\theta)$. Assume that $X(\theta) = h_T(\vec{Y}_T) I(T < \infty)$ (with T a stopping time), so that $\alpha(\theta) = E_\theta \{h_T(\vec{Y}_T); T < \infty\}$. Then, (3.8) yields

$$\alpha'(\theta_0) = E_{\theta_0} \{h_T(\vec{Y}_T) H(\theta_0); T < \infty\}, \quad (3.10)$$

where $H(\theta_0) = \mu'(\theta_0, Y_0)/\mu(\theta_0, Y_0) + \sum_{k=0}^{T-1} P'(\theta_0, Y_k, Y_{k+1})/P(\theta_0, Y_k, Y_{k+1})$. In certain settings, the estimator suggested by (3.10) may have a large variance (e.g. rare event simulation). For such problems, suppose that we select g to satisfy the positivity conditions stated earlier. Then

$$\alpha'(\theta_0) = E_g \{h_T(\vec{Y}_T) H(\theta_0); T < \infty\}, \quad (3.11)$$

where $H(\theta_0) = \mu(\theta_0, Y_0) \prod_{k=0}^{T-1} P(\theta_0, Y_k, Y_{k+1}) / g(\vec{Y}_T) \cdot [\mu'(\theta_0, Y_0)/\mu(\theta_0, Y_0) + \sum_{k=0}^{T-1} P'(\theta_0, Y_k, Y_{k+1}) / P(\theta_0, Y_k, Y_{k+1})]$. In a "rare event" setting, one would typically choose g so as to bias the system to force the occurrence of more rare events.

(3.12) EXAMPLE. In this example, we assume that under P_θ , Y is a Markov chain with non-stationary transition probabilities, so that $P_\theta \{Y_{k+1} = y_{k+1} | Y_k = y\} = P_k(\theta, y_k, y_{k+1})$. Then, if $\alpha(\theta) = E_\theta \{h_T(\vec{Y}_T); T < \infty\}$, (3.8) yields

$$\alpha'(\theta_0) = E_{\theta_0} \{h_T(\vec{Y}_T) H(\theta_0); T < \infty\}$$

where $H(\theta_0) = \mu'(\theta_0, Y_0)/\mu(\theta_0, Y_0) + \sum_{k=0}^{T-1} P'_k(\theta_0, Y_k, Y_{k+1})/P(\theta_0, Y_k, Y_{k+1})$; the obvious analog of (3.11) can also be written down.

4. LIKELIHOOD RATIO DERIVATIVE ESTIMATION IN CONTINUOUS TIME

This section is devoted to generalizing the ideas of Section 3 to continuous-time discrete-event dynamical systems. We view $X(\theta, \omega)$ as a sample performance measure associated with a continuous-time process ($Y = Y(t) : t \geq 0$) taking values in a discrete state space S . The process Y is assumed to be piece-wise constant with jump times S_1, S_2, \dots ($S_n \rightarrow \infty$ as $n \rightarrow \infty$). Hence, if $S_0 = 0$ and $Y_n = Y(S_n)$, we may write

$$Y(t) = \sum_{n=0}^{\infty} Y_n I(S_n \leq t < S_{n+1}).$$

Let $\Delta_n = S_{n+1} - S_n$ and put $Z_n = (Y_n, \Delta_n)$. We suppose that $\Omega = \hat{S} \times \hat{S} \times \dots$ where $\hat{S} = S \times [0, \infty)$ and that Z_n is the co-ordinate r.v. $Z_n(\omega) = \omega_n$ for $\omega = (\omega_0, \omega_1, \dots) \in \Omega$.

In order to proceed in parallel with the development of Section 3, we shall require that the distributions P_θ on Ω have the property that there exist measures μ_0, μ_1, \dots such that

$$\begin{aligned} P_\theta\{Z_0 \in dz_0\} &= p_0(\theta, z_0)\mu_0(dz_0) \\ P_\theta\{Z_{n+1} \in dz_{n+1} | \bar{Z}_n = \bar{z}_n\} &= p_n(\theta, \bar{z}_n, z_{n+1})\mu_n(\bar{z}_n, dz_{n+1}) \end{aligned}$$

where $\bar{Z}_n = (Z_0, \dots, Z_n)$ and $\bar{z}_n = (z_0, \dots, z_n) \in \hat{S} \times \dots \times \hat{S} = \Omega_n$ (($n + 1$) times). Then, analogously to (3.2), we may write

$$\begin{aligned} P_\theta\{\bar{Z}_n \in d\bar{z}_n\} &= \\ p_0(\theta, z_0) \prod_{k=0}^{n-1} p_k(\theta, \bar{z}_k; z_{k+1})\mu_n(d\bar{z}_n) & \quad (4.1) \end{aligned}$$

where $\mu_n(d\bar{z}_n) = \mu_0(dz_0) \prod_{k=1}^{n-1} \mu_k(\bar{z}_k, dz_{k+1})$.

Suppose now that we consider a performance measure $X(\theta)$ that is a function of the path up to horizon T ; this obviously includes any performance measure that depends on Y up to time S_{T+1} . As in Section 3, we require that T be a stopping time with respect to $Z = (Z_n : n \geq 0)$ i.e. for each $m \geq 0$, $I(T = m) = k_m(\bar{Z}_m)$ for some function k_m . Then, the performance measure $X(\theta)$ may be written in the form

$$\begin{aligned} X(\theta) &= \sum_{k=0}^{\infty} h_k(\theta, \bar{Z}_k) I(T = k) \\ &= h_T(\bar{Z}_T) I(T < \infty). \end{aligned}$$

Let $\Omega_T = \cup_{m=0}^{\infty} \{\bar{z}_m \in \Omega_m : k_m(\bar{z}_m) = 1\}$ and note that for $\bar{z}_T = (z_0, \dots, z_T) \in \Omega_T$, we may extend (4.1) to

$$\begin{aligned} P_\theta\{\bar{Z}_T \in d\bar{z}_T\} &= \\ p_0(\theta, z_0) \prod_{k=0}^{T-1} p_k(\theta, \bar{z}_k; z_{k+1})\mu_T(d\bar{z}_t) & \end{aligned}$$

where $\mu_T(d\bar{z}_T) = \mu_0(dz_0) \prod_{k=0}^{T-1} \mu_k(\bar{z}_k, dz_{k+1})$. By arguing identically as in Section 3, we obtain the following continuous-time generalization of (3.7). Suppose g is chosen as a non-negative function on Ω_T having the property that $\int_{\Omega_T} g(\bar{z}_T)\mu_T(d\bar{z}_T) = 1$ and $p_0(\theta_0, z_0) \prod_{k=0}^{T-1} p_k(\theta_0, \bar{z}_k, z_{k+1}) > 0$ implies that $g(\bar{z}_T) > 0$ for $\bar{z}_T \in \Omega_T$. Then, if $E_g(\cdot)$ is the expectation operator associated with $P(d\bar{z}_T) = g(\bar{z}_T)\mu(d\bar{z}_T)$, we obtain the derivative representation

$$\alpha'(\theta_0) = E_{\theta_0} X'(\theta_0) + E_g X(\theta_0) H(\theta_0)$$

for $\alpha(\theta) = E_\theta\{h(\theta, \bar{Z}_T); T < \infty\}$, where

$$\begin{aligned} H(\theta_0) &= p_0(\theta_0, z_0) \prod_{k=0}^{T-1} p_k(\theta_0, \bar{z}_k; z_{k+1}) / g(\bar{z}_T) \\ &\cdot \left[\frac{p'_0(\theta_0, z_0)}{p_0(\theta_0, z_0)} + \sum_{k=0}^{T-1} \frac{p'_k(\theta_0, \bar{z}_k; z_{k+1})}{p_k(\theta_0, \bar{z}_k; z_{k+1})} \right]. \quad (4.2) \end{aligned}$$

As in Section 3, one possible choice for g is $g(\bar{z}_T) = p_0(\theta_0, z_0) \prod_{k=0}^{T-1} p_k(\theta_0, \bar{z}_k; z_{k+1})$, in which case P is identical to P_{θ_0} , yielding

$$\alpha'(\theta_0) = E_{\theta_0}[X'(\theta_0) + X(\theta_0)H(\theta_0)] \quad (4.3)$$

where

$$H(\theta_0) = \frac{p'_0(\theta_0, Z_0)}{p_0(\theta_0, Z_0)} + \sum_{k=0}^{T-1} \frac{p'_k(\theta_0, \vec{Z}_k; Z_{k+1})}{p_k(\theta_0, \vec{Z}_k; Z_{k+1})}$$

$$\alpha'(\theta_0) = E_{\theta_0}[h(Y(s) : 0 \leq s \leq t) H(\theta_0)]$$

where

We shall now illustrate these formulae with some examples.

(4.4) EXAMPLE. Suppose that under P_θ , Y is a continuous-time Markov chain with initial distribution $\mu(\theta)$ and generator $Q(\theta)$. Assume that $X(\theta) = h(Y(s) : 0 \leq s \leq t)$. Then, $X(\theta)$ can be represented as $X(\theta) = \bar{h}(Z_0, Z_1, \dots, Z_T)$ where T is the stopping time $T = \inf\{n \geq 0 : \sum_{k=0}^n \Delta_k \geq t\}$. Set $z_n = (y_n, t_n)$ (recall that $z_n \in \bar{S} = S \times [0, \infty)$). Then,

$$P_\theta\{Z_0 \in dz_0\} = p_0(\theta, z_0) \mu_0(dz_0)$$

where $p_0(\theta, y_0, t_0) = \mu(\theta, y_0) q(\theta, y_0) \exp(-q(\theta, y_0)t_0)$, $q(\theta, y) = -Q(\theta, y, y)$, and $\mu_0(dz_0)$ is the product of counting measure and Lebesgue measure. Furthermore,

$$P_\theta\{Z_{n+1} \in dz_{n+1} | \vec{Z}_n = \vec{z}_n\} = \\ p_n(\theta, \vec{z}_n; z_{n+1}) \mu_n(\vec{z}_n, dz_{n+1})$$

where $p_n(\theta, \vec{z}_n; z_{n+1}) = Q(\theta, y_n, y_{n+1}) q(\theta, y_{n+1}) \exp(-q(\theta, y_{n+1})t_{n+1}) / q(\theta, y_n)$ and $\mu_n(\vec{z}_n, dz_{n+1})$ is again the product of counting measure and Lebesgue measure. Formula (4.3) now becomes

$$\alpha'(\theta_0) = E_{\theta_0}[h(Y(s) : 0 \leq s \leq t) H(\theta_0)]$$

where

$$H(\theta_0) = \frac{\mu'(\theta_0, Y_0)}{\mu(\theta_0, Y_0)} + \sum_{k=0}^{T-1} \frac{Q'(\theta_0, Y_k, Y_{k+1})}{Q(\theta_0, Y_k, Y_{k+1})} \\ + \frac{q'(\theta_0, Y_T)}{q(\theta_0, Y_T)} - \sum_{k=0}^T q'(\theta_0, Y_k) \Delta_k.$$

(4.5) EXAMPLE. Suppose that under P_θ , Y is a semi-Markov process with initial distribution $\mu(\theta)$, jump matrix $R(\theta)$, and holding time distributions $(F(\theta, x, dt) : x \in S)$. Suppose that for each x , $F(\theta, x, dt) = f(\theta, x, t)\mu(x, dt)$ for some measure μ . Assuming that $X(\theta) = h(Y(s) : 0 \leq s \leq t)$, we again put $T = \inf\{n \geq 0 : \sum_{k=0}^n \Delta_k \geq t\}$. Formula (4.3) becomes

$$H(\theta_0) = \frac{\mu'(\theta_0, Y_0)}{\mu(\theta_0, Y_0)} + \sum_{k=0}^{T-1} \frac{R'(\theta_0, Y_k, Y_{k+1})}{R(\theta_0, Y_k, Y_{k+1})} \\ + \sum_{k=0}^T \frac{f'(\theta_0, Y_k, \Delta_k)}{f(\theta_0, Y_k, \Delta_k)}.$$

(4.6) EXAMPLE. In this example, we show that (4.3) easily handles the case where the process is non-time homogeneous. In particular, suppose that under P_θ , Y is a non-time homogeneous continuous-time Markov chain with initial distribution $\mu(\theta)$ and time-dependent generator $Q(\theta, t)$. Then,

$$P_\theta\{Y_{n+1} = y, \Delta_{n+1} \in dt | \vec{Z}_n\} \\ = \frac{Q(\theta, S_{n+1}, Y_n, y)}{q(\theta, S_{n+1}, Y_n)} q(\theta, S_{n+1} + t, y) \\ \exp\left(-\int_0^t q(\theta, S_{n+1} + u, y) du\right) dt$$

where $q(\theta, t, y) = -Q(\theta, t, y, y)$. Suppose that $X(\theta) = h(Y(s) : 0 \leq s \leq t)$. If we put $T = \inf\{n \geq 0 : \sum_{k=0}^n \Delta_k \geq t\}$, then (4.3) takes the form

$$\alpha'(\theta_0) = E_{\theta_0}[h(Y(s) : 0 \leq s \leq t) H(\theta_0)]$$

where

$$H(\theta_0) = \frac{\mu'(\theta_0, Y_0)}{\mu(\theta_0, Y_0)} + \sum_{k=0}^{T-1} \frac{Q'(\theta_0, S_{k+1}, Y_k, Y_{k+1})}{Q(\theta_0, S_{k+1}, Y_k, Y_{k+1})} \\ + \frac{q'(\theta_0, S_{T+1}, Y_T)}{q(\theta_0, S_{T+1}, Y_T)} - \sum_{k=0}^T \int_{S_k}^{S_{k+1}} q'(\theta_0, t, Y_k) dt.$$

(4.7) EXAMPLE. We now suppose that Y is a generalized semi-Markov process (GSMP) under P_θ ; see GLYNN (1983) for further details on GSMP's. Let E be the event set of the GSMP. The initial state of the GSMP is chosen according to the distribution $\mu(\theta)$, whereas the initial clock readings are chosen from the distributions $F(\theta, e, dt)$, for $e \in E$.

When clock e initiates a transition from state y , the next state is chosen from the mass function $p(\theta, \cdot; y, e)$. Typically, when the GSMP enters a new state, certain clocks need to be stochastically reset. We assume that the distribution used to reset clock e' in state y' when a transition just occurred from state y with clock e as triggering event is given by $F(\theta, e', y', e, y, dt)$. We require that there exist measures $\mu(e, dt), \mu(e', y', e, y, dt)$ such that

$$\begin{aligned} F(\theta, e', y', e, y, dt) \\ = f(\theta, e', y', e, y, t), \mu(e', y', e, y, dt) \end{aligned} \quad (4.8)$$

$$F(\theta, e, dt) = f(\theta, e, t)\mu(e, dt).$$

In a strict sense, the analysis of this section does not apply to GSMP's, since the appropriate state descriptor for a GSMP includes the value of all the clock readings. Such a state descriptor can not typically be encoded as an element of $\hat{S} = S \times [0, \infty)$. However, a close examination of the analysis given earlier shows that the essential feature was that (Y_n, Δ_n) be representable as a simple function of the process Z_n ; Z_n need have no structure beyond (4.1). In particular, Z_n need not be an element of \hat{S} . In the GSMP setting, the natural candidate for Z is the tuple $Z_n = (Y_n, C_n)$, where C_n is the vector that describes the residual amount of time left on each of the clocks that are active in state Y_n . Clearly, Δ_n is a simple function of Z_n (in a GSMP with unit speeds, Δ_n is just the minimal element in C_n); furthermore, under (4.8), the distribution P_θ for Z_n can be written in the form (4.1).

Let $N(y'; y, e)$ be the set of clocks active in y' that need to be stochastically re-set when a transition from y just occurred with event e as the trigger. We further define $e^*(c)$ to be the index of the triggering event associated with clock vector c ; we assume e^* is uniquely defined for each c . Suppose $X(\theta) = h(Y(s) : 0 \leq s \leq t)$. If we put $T = \inf\{n \geq 0 : \sum_{k=0}^n \Delta_k \geq t\}$, it is easily verified that (4.3) takes the form

$$\alpha'(\theta_0) = E_{\theta_0}[h(Y(s) : 0 \leq s \leq T)H(\theta_0)]$$

where

$$H(\theta_0)$$

$$\begin{aligned} &= \frac{\mu'(\theta_0, Y_0)}{\mu(\theta_0, Y_0)} + \sum_{k=0}^{T-1} \frac{p'(\theta_0, Y_{k+1}; Y_k, e^*(C_k))}{p(\theta_0, Y_{k+1}; Y_k, e^*(C_k))} \\ &+ \sum_e \frac{f'(\theta_0, e, C_{0e})}{f(\theta_0, e, C_{0e})} + \sum_{k=1}^T \\ &\quad \sum_{e \in N(Y_k; Y_{k-1}, e^*(C_{k-1}))} \frac{f'(\theta_0, e, Y_k, e^*(C_{k-1}), Y_{k-1}, C_{ke})}{f(\theta_0, e, Y_k, e^*(C_{k-1}), Y_{k-1}, C_{ke})}. \end{aligned}$$

The above examples serve to illustrate the great variety of stochastic processes to which likelihood ratio derivative estimation may be applied.

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